ALGORITHMS FOR OPTIMAL

NUMERICAL QUADRATURE BASED

ON SIGNAL CLASS MODELS

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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

A framework is presented for constructing various types of numerical quadrature algorithms which take into account the a-priori known or estimated properties of the signal being processed. This is done by appropriately modeling the signal class to which such a signal belongs. Both linear and nonlinear signal class models are considered and wide use of generalized spline theory is made. For the nonlinear case, a new type of nonlinear generalized spline is defined.

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CONTENTS

1. INTRODUCTION

Let g denote a complex-valued function of the real variable t, integrable with respect to a Lebesgue Stieltjes measure μ on an interval I. By the "quadrature" of g on I we mean the value of the integral

$$Q(g) = \int_I g(t')\, d\mu(t'). \tag{1}$$

By "numerical quadrature" of g we mean an (approximate) evaluation $Q_N(g)$ of $Q(g)$ by means of a numerical algorithm based on a set of samples of g on I and possibly on some of the derivatives of g at the endpoints of I.

Quadrature evaluations occur in important applications. Some of the applications that we shall consider are:

(a) <u>Ordinary integration</u> of g over an interval I (μ is then the ordinary Lebesgue measure on the real line);

(b) Calculation of the <u>nth. moment</u> of g, where g is a mass density, a charge density, or a probability density over I, thus

$$Q(g) = \int_I (t')^n\, g(t')\, dt', \tag{2}$$

where n is an arbitrary nonnegative integer;

(c) <u>Convolution</u> of a signal g with an impulse response h of a dynamical system, thus

$$Q(g) = \int_I h(t-t')\, g(t')\, dt'; \tag{3}$$

and (d) the Fourier transform of a signal g, thus

$$Q(g) = \int_{-\infty}^{\infty} e^{-j2\pi f t'} g(t') \, dt'. \qquad (4)$$

The main thrust of the work reported here is the use of "physical models" for generating "strictly numerical" quadrature algorithms as follows: We assume that g is generated by a dynamical system driven by an imput u whose energy is finite over the interval I, i.e. $u \in L^2(I)$. Through such a selection of a dynamical model it is possible to incorporate a-priori information about g into the design of an algorithm for the numerical quadrature of g.

Our model for the generation of g is of the form (See Fig.1):

$$\tilde{F}(g) = F(g, g', \ldots, g^{(n)}) = u, \quad ' = d/dt, \qquad (5)$$

where $\tilde{F}$ is a general nth. order differential operator. In the linear case we assume

$$\tilde{F}(g) = \sum_{k=0}^{n} a_k g^{(k)} = \left(\sum_{k=0}^{n} a_k D^k \right) g \triangleq L(D) g, \quad D = d/dt, \qquad (6)$$

where $a_n = 1$, and a_k, $k = 0, \ldots, n-1$, are real constants. In the nonlinear case, we assume that F is a smooth function of its $(n+1)$ arguments $g, g', \ldots, g^{(n)}$, having continuous partials with respect to these variables up to order n.

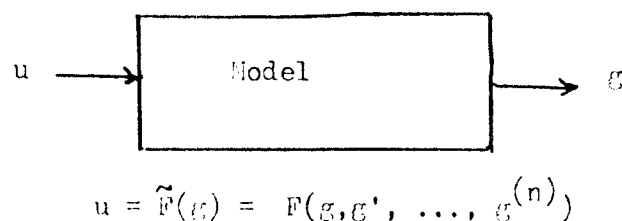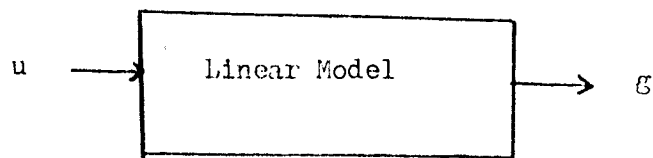$$u = \tilde{F}(g) = F(g, g', \ldots, g^{(n)})$$

Fig. 1 (a) General Operator Model

In both the linear and nonlinear cases, numerical quadrature algorithms will be obtained as solutions of an optimization problem.

$$u \longrightarrow \boxed{\text{Linear Model}} \longrightarrow g$$

$$u = \widetilde{F}(g) = L(D)\, g = \left(\sum_{k=0}^{n} a_k D^k \right) g, \quad D = d/dt$$

Fig.1(b)   Linear Operator Model

In Section 2, we consider the case of a linear source model for g and, in section 3, we extend the theory to the nonlinear case.

Numerical simulations performed at Rice show the merits of the present approach and they will be described separately.

2. QUADRATURE BASED ON LINEAR MODELS

As we shall see in subsection 2.1, linear models lead to solutions based on generalized splines. Considerable amount of research on quadrature formulas based on splines has been done by Schoenberg [1] [2], Sard [3], and Golomb [4]. In what follows, we recast some of this spline theory in the language of dynamic models.

In subsections 2.2 through 2.5, we show that such models lead to appropriate "windows" for use in the numerical evaluation of ordinary integrals, moments, convolutions, and Fourier transforms. In what we have just stated, we have assumed that the model generating g is given to us. If it is unknown, we show, in subsection 2.6, how to retrieve it from the data using a maximum entropy approach.

2.1. Fundamentals of Spline Based Solutions

Let $H_n^2(I)$ denote the Sobolev space of complex-valued functions g on $I = [a,b]$ such that $g^{(k)}$, $k = 0, 1, \ldots, n-1$, are absolutely continuous and $g^{(n)} \in L^2(I)$. We will denote by $\hat{H}_n^2(I)$ the closed subspace of $H_n^2(-\infty, \infty)$ defined by

$$\hat{H}_n^2(I) = \left\{ g \in H_n^2(-\infty, \infty) : g(t) = 0, \ t < a, \ t > b; \ g^{(k)}(a) = g^{(k)}(b) = 0, \right.$$

$$1, \ldots, n-1; \text{ the restriction of } g \text{ to } I$$

$$\left. \text{belongs to } H_n^2(I) \right\}. \tag{7}$$

Also, let $L(D)$ be the linear operator defined by (6), i.e.

$$L(D) = D^n + \sum_{k=0}^{n-1} a_k D^k . \tag{8}$$

We will assume that the signal g under consideration (whose quadrature is to be obtained) satisfies the following conditions:

(i) $g \in \hat{H}_n^2 (I)$;

(ii) we are given a set of complex numbers $r_1, \ldots, r_N$ and a mesh

$$a = t_0 < t_1 < \ldots \qquad < t_N < t_{N+1} = b, \tag{9}$$

with respect to which g satisfies the interpolating constraints

$$g(t_i) = r_i, \quad i = 1, \ldots, N; \tag{10}$$

(iii) g belongs to the ellipsoidal class

$$\left\{ g \in \hat{H}_n^2(I) : \ \left\| L(D) \ g \right\|_{L^2_{(-\infty,\infty)}} \leq \gamma \right\} , \tag{11}$$

where γ is some positive constant, and $L(D)$ is assumed given.

If g satisfies all the above three conditions, we will write

$$g \in \mathcal{X} . \tag{12}$$

Note that $\hat{H}_n^2 (I)$ constitutes a Hilbert space under the inner product

$$(g,h)_{\hat{H}_n^2(I)} = \int_a^b \Big(L(D) \ g^*(t) \Big)\Big(L(D)h(t) \Big) dt, \quad * = \text{complex conj.} \tag{13}$$

We will use the folllowing two wellknown results [4] .

Proposition 1. The min-max problem

$$\min_{g \in \hat{H}_n^2(I)} \ \max_{\tilde{g} \in \mathcal{X}} \ \left\| g - \tilde{g} \right\|_{\hat{H}_n^2(I)} \tag{14}$$

has a unique solution $\hat{g}$ which is the **L-spline** defined by the set of equations and conditions:

$$L(-D)\ L(D)\ \hat{g}(t) = 0,\quad t_i < t < t_{i+1},\quad i = 0, \ldots, N; \tag{15a}$$

$$\hat{g}(t_i) = r_i,\quad i = 1, \ldots, N; \tag{15b}$$

$$\hat{g} \in C^{2n-2}(I);\quad g \in H_n^2(I); \tag{15c}$$

where $C^k(I)$ = space of functions on I with continuous k^{th} derivatives.

The u corresponding to such a g is obtained simply by the relationship

$$u = L(D)\ \hat{g}. \tag{16}$$

$\underline{\text{Proposition 2}}$. Let Φ be a continuous linear functional on $\hat{H}_n^2(I)$. The min-max problem

$$\min_{g \in \hat{H}_n^2(I)}\ \max_{\tilde{g} \in \chi}\ |\Phi(g) - \Phi(\check{g})| \tag{17}$$

has a unique solution $\widehat{\Phi(g)}$ given by

$$\widehat{\Phi(g)} = \Phi(\hat{g}), \tag{18}$$

where $\hat{g}$ is L-spline of Proposition 1.

Recognizing that for $g \in H_n^2(I)$ the quadrature

$$Q(g) = \int_a^b g(t)\ d\mu(t) \tag{19}$$

is a continuous linear functional on $\hat{H}_n^2(I)$, Proposition 2 provides us with a

technique for calculating numerical quadrature $Q_N(g)$ as a best estimate $Q(\hat{g})$ of $Q(g)$ on the basis of the data $\hat{g}^{(k)}(a) = \hat{g}^{(k)}(b) = 0$, $k = 0,\ldots,$ n-1, $\hat{g}(t_i) = r_i$, $i = 1,\ldots,N$, and the "physical model" that generates $\hat{g}$, described by the dynamical system

$$L(D)\ \hat{g}(t) = \hat{u}(t). \tag{20}$$

The solution is to interpolate the data by the spline associated with the operator L and then perform the quadrature on this spline.

By way of example, suppose we model g as the output of a low-pass filter with half-power frequency equal to one (See Fig. 2). We then have

$$L(D)\ =\ D + 1, \tag{21}$$

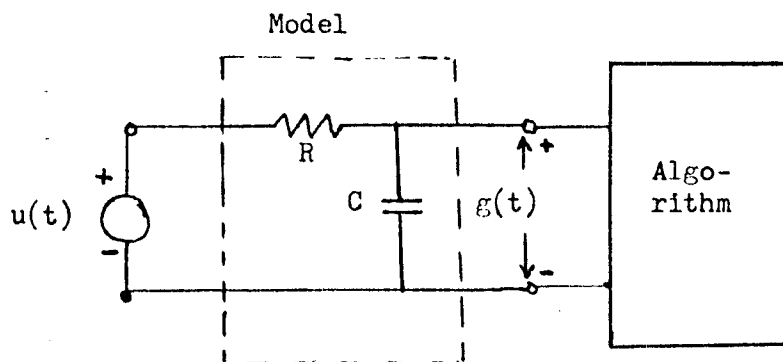and the roots of the characteristic equations associated with $L(D)$ and $L(-D)$ are respectively -1 and 1.

Fig. 2. Network Model for Basing Optimal Numerical
Quadrature Algorithm

So we have:

$$g(t) = a^+_i \, e^{-t} + a^-_i \, e^t \, , \quad t_i < t < t_{i+1} \, ,$$

$$i = 0, 1, \ldots, N \, , \tag{22}$$

where the constants a^+_i and a^-_i are associated with the homogeneous solutions pertaining to $L(D)$ and $L(-D)$. These constants are determined, according to (15a) through (15c), by the requirements that g satisfy the interpolating constraints and the boundary conditions, and that g be continuous on I.

In the general case in which the characteristic equation

$$L(s) = 0 \tag{23}$$

associated with the operator $L(D)$ has n distinct roots $s_1, \ldots, s_n$, (22) generalizes to

$$g(t) = \sum_{j=1}^{n} \left[a^+_{ij} \, e^{s_j t} + a^-_{ij} \, e^{-s_j t} \right] \, , \quad t_i < t < t_{i+1} \, ,$$

$$i = 0, 1, \ldots, N \, , \tag{24}$$

where again the constants a^+_{ij} and a^-_{ij} are determined by the requirement that the interpolating and boundary constraints be satisfied in addition to the requirement that the derivatives of g up to the order $2n-2$ be continuous at the knots.

If (23) has a repeated root say s_k of multiplicity ν_k, the expression inside the square brackets in (24) for that particular root is replaced by

$$\left[\sum_{p=0}^{\nu_k - 1} (a_{ikp}^+ \, t^p \, e^{s_j t} + a_{ikp}^- \, (-t)^p \, e^{-s_j t}) \right],$$ (25)

where a_{ikp}^+ and a_{ikp}^- are suitable constants that depend on the data and other conditions as mentioned above.

A set of <u>basis functions</u> which makes the dependence of g on the data transparent is the so-called "<u>cardinal spline basis</u>" [5] (also called "fundamental spline basis" [6]). This basis, which we denote by B, is the set of splines $b_1(t),\ldots,b_N(t)$ satisfying 15(a) through 15(c) with the data satisfying $r_i = \delta_{ij}$ (=kronecker delta) for the spline b_j. Thus the spline b_j has zero values at all the knots except at the jth. knot where it has value of unity. It vanishes outside $[a,b]$. The sketches of Fig. 3 exhibit the shapes of these basis functions. They look and act very much like sinc functions and they apply to a finite set of samples (rather than an infinite set like the sinc functions).
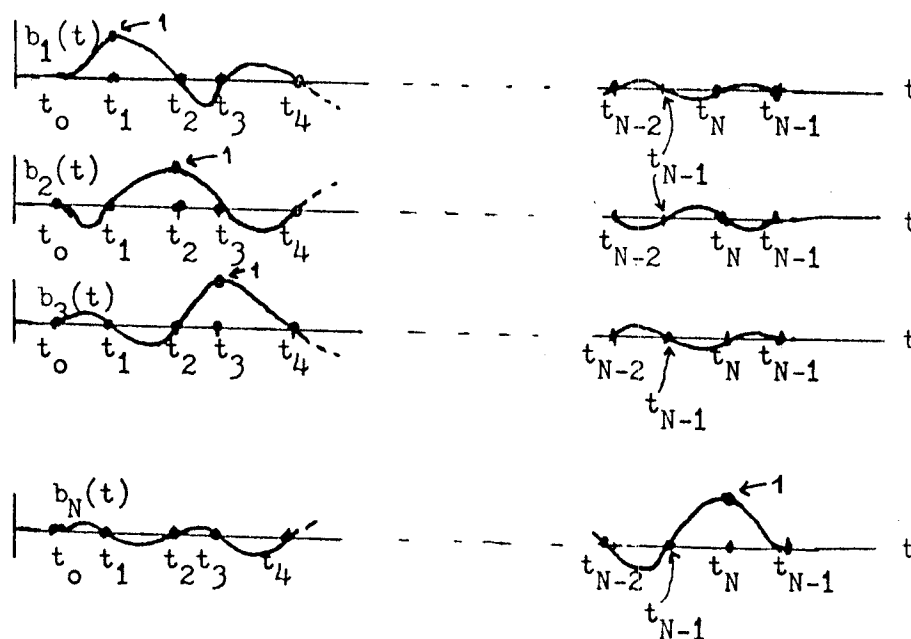
Fig. 3. Sketches of Cardinal Spline Basis Functions

In terms of the basis elements of B, $\hat{g}$ can be represented as

$$\hat{g}(t) = \sum_{i=1}^{N} g(t_i)\, b_i(t)$$

$$= \sum_{i=1}^{N} r_i\, b_i(t). \tag{26}$$

We will use this representation of $\hat{g}$ in the following subsections.

Summarizing the developments in this subsection, we claim that we have given all the details required to represent and calculate the entities needed for the quadrature problems described below. They were used in the numerical simulations performed on our computers.

2.2. Ordinary Integration

The first application that we shall consider is the numerical integration

$$Q(g) = \int_{t_1}^{t_N} g(t)\, dt, \tag{27}$$

based on samples of g given by (10) and on the other conditions stated previously.

Representing our optimal estimate $\hat{g}$ of g by means of the cardinal spline basis functions given by (26), we obtain the formula for the "model based" numerical integration corresponding to (27):

$$Q_N(g) = \sum_{i=1}^{N} w_i\, g(t_i) = \sum_{i=1}^{N} w_i\, r_i , \tag{28a}$$

where

$$w_i = \int_{t_1}^{t_N} b_i(t)\, dt \ , \quad i = 1, \dots, N. \tag{28b}$$

2.3. Evaluation of Moments

We remind the reader that in this and in the following subsections, we assume the signal g to vanish outside the interval (a,b). This interval is of course allowed to be of infinite length if necessary, by setting $a = -\infty$ and/or $b = \infty$.

An optimal algorithm for the numerical evaluation of the kth. moment now follows from the preceding theory to be

$$Q_N(g) = \sum_{i=1}^{N} w_i\, g(t_i) = \sum_{i=1}^{N} w_i\, r_i, \tag{29a}$$

where

$$w_i = \int_I t^k\, b_i(t)\, dt, \quad i = 1, \dots, N. \tag{29b}$$

2.4. Convolution

Our model-based optimal numerical scheme for convolution of g with an impulse response h is

$$Q_N(h \bullet g)\,(t) = \sum_{i=1}^{N} w_{it}\, g(t_i) = \sum_{i=1}^{N} w_{it}\, r_i \ , \tag{30a}$$

$$w_{1t} = \int_I h(t-t') \, b_1(t') \, dt', \quad i = 1, \ldots, N. \tag{30b}$$

2.5. Fourier Transforms and Filter Transfer Functions

In the same fashion as in the preceding subsections, we derive our model-based algorithm for the calculation of the Fourier transform of g by

$$Q_N(g)(\omega) = \sum_{i=1}^{N} w_{1\omega} \, g(t_1) = \sum_{i=1}^{N} w_{1\omega} r_1, \tag{31a}$$

where

$$w_{1\omega} = \int_{-\infty}^{\infty} b_1(t) \, e^{-j\omega t} \, dt, \quad i = 1, \ldots, N. \tag{31b}$$

Note that in the special case in which the sampling instants are equidistant, if we set

$$b_1(t) = \delta(t - t_1),$$

(31a) (if we consider appropriate discrete values of ω) becomes the discrete Fourier transform of the data. Thus we see that the algorithm that we proposed is a flexible "model-based" extension of the DFT algorithm.

In the case in which g is the impulse response of a filter, we conclude that (31a) and (31b) constitute an optimal algorithm for the derivation of its transfer function in terms of the samples of the impulse response.

2.6. Model Identification by a Maximum Entropy Approach

Thus far, the differential operator L(D) describing the model was assumed known. In general, this may not be the case, and one would like to develop a methodology for determining L(D) from the data and other

prior information. Precisely, this may be formulated as follows:

Problem. Find the constants $a_0, a_1, \ldots, a_{n-1}$ in the differential operator (8) from the data $r_1, \ldots, r_N$.

The identification procedure that we propose applies to uniformly sampled data and is as follows. We assume that the samples $\{r_k\}$ result from an auto-regressive process.

$$r_{k+n} + a_{n-1} r_{k+n-1} + \ldots + a_1 r_{k+1} + a_0 r_k = u_k, \quad k = 1, \ldots, N-n, \quad (33)$$

where u_k is a white noise process. The rationale for this assumption is that it constitutes a discrete stochastic version of equation (6).

From $r_1, \ldots r_N$, we compute n samples of the sample autoavariance $\hat{R}_g(\ell)$, $= 0, \ldots n-1$. From these, the coefficients a_j may be obtained by requiring that the Yule-Walker equations [7] be satisfied by $\hat{R}_g$, i.e.

$$\sum_{j=0}^{n-1} a_j \hat{R}_g(j-\ell) = -\hat{R}_g(n-\ell), \quad \ell = 1, \ldots, n . \quad (34)$$

The coefficients $\{a_j\}$ can also be obtained for the process (33) using the maximum entropy method in a standard way [8].

3. QUADRATURE BASED ON NONLINEAR MODELS

We now propose a generalization of the preceding theory for the case in which the signal g is assumed to be generated by the nonlinear model (5).

We assume that g satisfies conditions (i) and (ii) stated at the top of page 5 and (instead of belonging to the ellipsoidal class (11)) belongs to the class

$$\Psi = \left\{ g \in \hat{H}_n^2 (I) : \| F(g,g' \ldots, g^{(n)}) \|_{L^2(-\infty, \infty)} \leq \tau \right\}, \qquad (35)$$

where the F is such that Ψ is a convex and symmetric set in $\hat{H}_n^2 (I)$ and, in addition, all nth order partials of F with respect to all its arguments are continuous.

We recall from the literature [4] [9] that in the linear case the solution $\hat{g}$ of (14) is also the solution of the minimum norm problem

$$\min_{g \in \hat{H}_n^2(I)} \| L(D)g \|_{L^2(I)}^2 . \qquad (36)$$

$$g(t_i) = r_i, i = 1, \ldots, N$$

By analogy, we seek the best estimate $\hat{g}$ of g in the nonlinear case as the solution of

$$\min_{g \in \hat{H}_n^2(I)} \| \tilde{F}(g) \|_{L^2(I)}^2 , \qquad (37)$$

$$g(t_i) = r_i, i = 1, \ldots N$$

where we recall that

$$\tilde{F}(g) = F(g, g', \ldots g^{(n)}) .$$ (38)

For simplicity in presentation let us assume that the underlying linear spaces are over the field of reals.

The solution $\hat{g}$ of (37) will be called a "nonlinear spline". Such $\hat{g}$ must satisfy [10]:

$$\delta \int_a^b F^2(\hat{g}, \hat{g}', \ldots, \hat{g}^{(n)}) \, dt = 0 ,$$ (39b)

$$\hat{g}(t_i) = r_i, \quad i = 1, \ldots, N .$$ (39b)

Performing the variation indicated in (39a) (under the fixed boundary conditions assumed earlier), we are led to the Euler equation (we omit the details of the derivation):

$$\sum_{k=0}^{n} \left(-\frac{d}{dt}\right)^k \left[F(\hat{g}, \hat{g}', \ldots, \hat{g}^{(n)}) \, \frac{\partial F(\hat{g}, \hat{g}', \ldots \hat{g}^{(n)})}{\partial \hat{g}^{(k)}} \right] = 0$$ (40)

Thus the nonlinear spline $\hat{g}$ is described by the nonlinear differential equation (40) in each of the subintervals $t_i < t < t_{i+1}$, $i = 0, 1, \ldots, N$, and by the conditions (15b) and (15c).

The optimal numerical quadrature based on the nonlinear model developed above is simply given by (19) with g replaced by $\hat{g}$ of the preceeding paragraph.

4. CONCLUSION

A physical modeling basis and framework have been provided for constructing various quadrature algorithms. For this purpose, both existing and new results on spline theory have been presented.

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